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The predicted heats of formation of DNAF,

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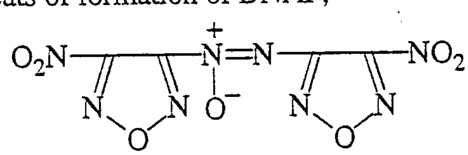

based on computational analyses, are: ΔH_f(gaseous) = 169 kcal/mole = 621 cal/g; ΔH_f(liquid) = 155 kcal/mole = 570 cal/g; ΔH_f(solid) = 137 kcal/mole = 504 cal/g.

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Dr. Richard S. Miller

Technical Report No. 85

PREDICTED HEATS OF FORMATION OF DNAF IN GASEOUS, LIQUID AND SOLID PHASES

by

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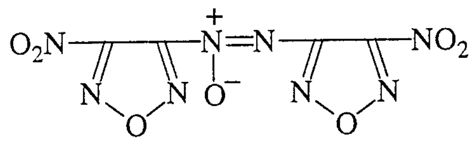
October 10, 1995

One of the compounds for which we have recently computed the gas phase heats of formation, ΔH_f(gaseous), is DNAF, **1** [1]. This was done using our density functional procedure [2].



DNAF, **1**

In response to interest expressed by the Air Force Armament Laboratory (Eglin AFB), we have now estimated the liquid and solid phase heats of formation of **1**. For this purpose, we needed the heats of vaporization, ΔH_{vap}, and sublimation, ΔH_{sub}, which we obtained using general correlations between these properties and computed quantities related to electrostatic potentials on molecular surfaces [3].

$$\Delta H_f(\text{liquid}) = \Delta H_f(\text{gaseous}) - \Delta H_{vap} \tag{1}$$

$$\Delta H_f(\text{solid}) = \Delta H_f(\text{gaseous}) - \Delta H_{sub} \tag{2}$$

We found ΔH_{vap} = 14 kcal/mole and ΔH_{sub} = 32 kcal/mole. Then,

$$\Delta H_f(\text{gaseous}) = 169 \text{ kcal/mole} = 621 \text{ cal/g}$$

$$\Delta H_f(\text{liquid}) = 155 \text{ kcal/mole} = 570 \text{ cal/g}$$

$$\Delta H_f(\text{solid}) = 137 \text{ kcal/mole} = 504 \text{ cal/g}$$

References

1. P. Politzer and M. E. Grice, Technical Report No. 78, Office of Naval Research, Contract No. N00014-95-1-0028, March 16, 1995.
2. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, J. Comp. Chem., **16**, 654 (1995).
3. M. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.